Modeling electrostatic potential of biological membranes

Lead scientist: Dr. Lin Li

Collaboration with Prof. Thereza Soares (Brazil)

Abstract: Many naturally occurring lipopolysaccharide membranes are asymmetric and the asymmetry reflects their biological function, particularly the distribution of the electrostatic potential across the membrane. Here we investigate four chemotypes of lipopolysaccharide membranes by a combined approach of molecular dynamics (MD) simulations and continuum electrostatics. It is demonstrated that Ca2+ ions, bridging the phosphate groups, play essential role for electrostatic potential distribution overcompensating for the negative potential generated by phosphate groups. A new tool for modeling the electrostatic potential profile along the axis of membrane, MEMPOT, was developed and implemented in DelPhi. Using MEMPOT and snap shots from MD simulations, the average inter-membrane potential was found to be positive for all chemotypes and to have complex profile. Comparing the snap shot average electrostatic potential profile and the profile obtained from either initial structure and a single snap shot, sets of effective dielectric constants (for lipid tails and phosphate regions respectively) were delivered according to the chemotypes and it was shown that their dielectric constants reflect the different flexibility of the chemotypes observed in MD simulations. In general the optimal dielectric for tail region is found to be always smaller than the same for the phosphare region, but the optimal values are chemotype specific. These findings provide rules of how to mimic conformational flexibility via chemotypes specific effective dielectric constants using a single structure in conjunction with the new DelPhi feature, the MEMPOT. In addition, the importance of taking into account water phase is also demonstrated.

Results (ongoing project):

(a) Potential z-axis distribution for lipid A chemotype